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{Bis[2-(diphenylphosphino)ethyl]phenylphosphine- κ^3P,P',P'' }chlorido-platinum(II) hexafluoridophosphate

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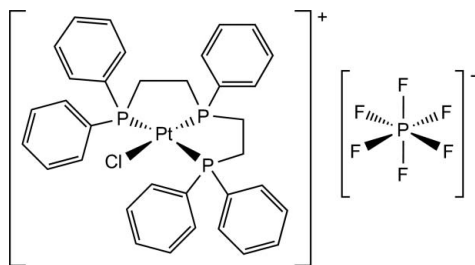
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 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; disorder in solvent or counterion; R factor = 0.020; wR factor = 0.049; data-to-parameter ratio = 13.6.

In the title compound, $[\text{PtCl}(\text{C}_{34}\text{H}_{33}\text{P}_3)]\text{PF}_6$, the Pt^{II} cation adopts a distorted square-planar PtClP_3 geometry, arising from the P,P',P'' -tridentate triphos ligand and a chloride ion. Four of the F atoms of the PF_6^- anion are disordered over two sets of positions in a 0.614 (17):0.386 (17) ratio.

Related literature

The corresponding complex with a Pd^{II} metal center is published concurrently (Vorce *et al.*, 2009). The corresponding Pt^{II} complex has been previously reported as a CuCl_2^- salt (Fernandez *et al.*, 2005). The corresponding complexes with both Pt^{II} and Pd^{II} have been previously reported as chloride and diphenyltetrachloridostannate(IV) salts (Sevillano *et al.*, 1999a; Garcia-Seijo *et al.*, 2001; Housecroft *et al.*, 1990). For other group 10–triphos complexes, see: Sevillano *et al.* (1999b); Müller *et al.* (2000); Aizawa *et al.* (2002); Bertinsson *et al.* (1983); Autissier *et al.* (2005); Fernandez *et al.* (2005); King *et al.* (1971).



Experimental

Crystal data

 $[\text{PtCl}(\text{C}_{34}\text{H}_{33}\text{P}_3)]\text{PF}_6$
 $M_r = 910.02$

 Monoclinic, $P2_1/c$
 $a = 11.3870$ (11) Å
 $b = 19.6221$ (18) Å
 $c = 16.4439$ (16) Å
 $\beta = 107.528$ (3)°
 $V = 3503.6$ (6) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 4.32$ mm⁻¹
 $T = 298$ K
 $0.50 \times 0.30 \times 0.10$ mm

Data collection

 Bruker SMART X2S diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 2008a)
 $T_{\text{min}} = 0.21$, $T_{\text{max}} = 0.65$

 21968 measured reflections
 6155 independent reflections
 5269 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.025$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.020$
 $wR(F^2) = 0.049$
 $S = 1.03$
 6155 reflections
 452 parameters

 204 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.58$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.41$ e Å⁻³

Table 1

Selected bond lengths (Å).

| | | | |
|--------|------------|---------|------------|
| Pt1—P2 | 2.2095 (8) | Pt1—P1 | 2.3185 (8) |
| Pt1—P3 | 2.3007 (8) | Pt1—Cl1 | 2.3434 (8) |

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT and XPREP (Bruker, 2008); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008b); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008b); molecular graphics: SHELXTL (Sheldrick, 2008b); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2993).

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supplementary materials

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{Bis[2-(diphenylphosphino)ethyl]phenylphosphine- κ^3P,P',P'' }chloridoplatinium(II) hexafluoridophosphate

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Comment

The crystal structure of the title compound, (I), consists of a $[\text{Pt}(\text{triphos})\text{Cl}]^+$ cation and disordered PF_6^- anion (Fig. 1). The cation shows a distorted square planar geometry (Table 1) around the metal center with a non-coordinating PF_6^- anion.

Experimental

The synthesis of (I) by a previously reported procedure (King, *et al.*, 1971). Crystals were grown by slow solvent evaporation of a saturated dichloromethane solution of (I).

Figures

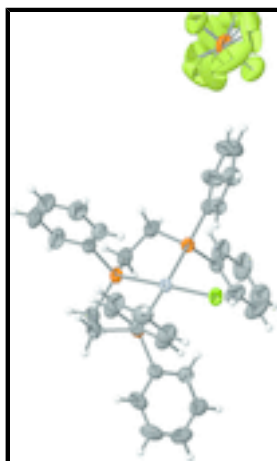


Fig. 1. The molecular structure of (I), with 50% probability displacement ellipsoids.

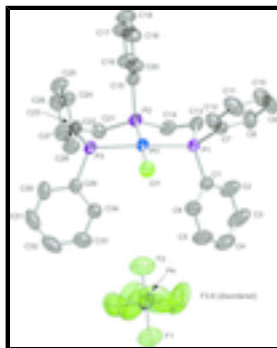


Fig. 2. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids. Hydrogen atoms are omitted for clarity.

{Bis[2-(diphenylphosphino)ethyl]phenylphosphine- κ^3P,P',P'']chloridoplatinium(II) hexafluoridophosphate

Crystal data

| | |
|--|---|
| [PtCl(C ₃₄ H ₃₃ P ₃)]PF ₆ | $F_{000} = 1784$ |
| $M_r = 910.02$ | $D_x = 1.725 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$ |
| Hall symbol: -P 2ybc | Cell parameters from 9957 reflections |
| $a = 11.3870 (11) \text{ \AA}$ | $\theta = 2.5\text{--}25.1^\circ$ |
| $b = 19.6221 (18) \text{ \AA}$ | $\mu = 4.32 \text{ mm}^{-1}$ |
| $c = 16.4439 (16) \text{ \AA}$ | $T = 298 \text{ K}$ |
| $\beta = 107.528 (3)^\circ$ | Plate, colorless |
| $V = 3503.6 (6) \text{ \AA}^3$ | $0.50 \times 0.30 \times 0.10 \text{ mm}$ |
| $Z = 4$ | |

Data collection

| | |
|--|--|
| Bruker SMART X2S diffractometer | 6155 independent reflections |
| Monochromator: graphite | 5269 reflections with $I > 2\sigma(I)$ |
| Detector resolution: $8.33 \text{ pixels mm}^{-1}$ | $R_{\text{int}} = 0.025$ |
| $T = 298 \text{ K}$ | $\theta_{\text{max}} = 25.1^\circ$ |
| ω scans | $\theta_{\text{min}} = 2.8^\circ$ |
| Absorption correction: multi-scan (SADABS; Sheldrick, 2008a) | $h = -13 \rightarrow 13$ |
| $T_{\text{min}} = 0.21, T_{\text{max}} = 0.65$ | $k = -18 \rightarrow 23$ |
| 21968 measured reflections | $l = -19 \rightarrow 19$ |

Refinement

| | |
|--|--|
| Refinement on F^2 | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.020$ | H-atom parameters constrained |
| $wR(F^2) = 0.049$ | $w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 1.641P]$ |
| $S = 1.03$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 6155 reflections | $(\Delta/\sigma)_{\text{max}} = 0.002$ |
| 452 parameters | $\Delta\rho_{\text{max}} = 0.58 \text{ e \AA}^{-3}$ |
| 204 restraints | $\Delta\rho_{\text{min}} = -0.41 \text{ e \AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. The PF₆ anion is disordered, showing alternate positions of the 4 F atoms F3—F6 when rotated about the axis F1—P4—F2. A second orientation for these equatorial positions was located. Based on the thermal parameters, additional positions are indicated, but were not modeled. To improve the quality of the fit for this anion, distance restraints (*SHELX SADI*) were added for the P—F bonds, as well as for the F—F interatomic distances. These account for 156 of the 204 restraints applied. The remaining restraints (*ISOR*) were applied to the anisotropic displacement parameters for the fluorine atoms.

Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ | Occ. (<1) |
|-----|---------------|--------------|--------------|----------------------------------|-----------|
| Pt1 | 0.139852 (10) | 0.364806 (6) | 0.374003 (7) | 0.03173 (5) | |
| Cl1 | 0.31867 (8) | 0.35123 (5) | 0.48942 (5) | 0.0498 (2) | |
| P1 | 0.22200 (7) | 0.43573 (4) | 0.29227 (5) | 0.03695 (19) | |
| P2 | -0.03648 (7) | 0.37743 (4) | 0.27189 (5) | 0.03518 (19) | |
| P3 | 0.03774 (7) | 0.28264 (4) | 0.42630 (5) | 0.03706 (19) | |
| C1 | 0.3286 (3) | 0.39017 (18) | 0.2487 (2) | 0.0417 (8) | |
| C2 | 0.3950 (4) | 0.3357 (2) | 0.2925 (3) | 0.0696 (12) | |
| H2 | 0.3851 | 0.3227 | 0.3444 | 0.084* | |
| C3 | 0.4758 (5) | 0.3003 (3) | 0.2602 (4) | 0.0929 (17) | |
| H3 | 0.5209 | 0.2641 | 0.2909 | 0.111* | |
| C4 | 0.4896 (4) | 0.3182 (3) | 0.1838 (3) | 0.0811 (14) | |
| H4 | 0.5422 | 0.2933 | 0.1614 | 0.097* | |
| C5 | 0.4268 (4) | 0.3724 (3) | 0.1397 (3) | 0.0809 (15) | |
| H5 | 0.4382 | 0.3850 | 0.0881 | 0.097* | |
| C6 | 0.3458 (4) | 0.4088 (2) | 0.1716 (2) | 0.0662 (12) | |
| H6 | 0.3030 | 0.4457 | 0.1413 | 0.079* | |
| C7 | 0.2923 (3) | 0.51580 (17) | 0.3367 (2) | 0.0448 (8) | |
| C8 | 0.3091 (4) | 0.5681 (2) | 0.2843 (3) | 0.0690 (12) | |
| H8 | 0.2889 | 0.5616 | 0.2257 | 0.083* | |
| C9 | 0.3563 (5) | 0.6303 (2) | 0.3202 (4) | 0.0815 (15) | |
| H9 | 0.3673 | 0.6653 | 0.2852 | 0.098* | |
| C10 | 0.3863 (4) | 0.6405 (2) | 0.4054 (4) | 0.0774 (15) | |
| H10 | 0.4162 | 0.6827 | 0.4283 | 0.093* | |
| C11 | 0.3726 (4) | 0.5886 (2) | 0.4579 (3) | 0.0774 (14) | |
| H11 | 0.3950 | 0.5954 | 0.5166 | 0.093* | |
| C12 | 0.3255 (3) | 0.5262 (2) | 0.4237 (3) | 0.0587 (10) | |
| H12 | 0.3162 | 0.4913 | 0.4595 | 0.070* | |

supplementary materials

| | | | | | |
|------|--------------|--------------|--------------|-------------|------------|
| C13 | 0.0924 (3) | 0.46082 (19) | 0.2000 (2) | 0.0480 (9) | |
| H13A | 0.0534 | 0.5012 | 0.2141 | 0.058* | |
| H13B | 0.1226 | 0.4718 | 0.1524 | 0.058* | |
| C14 | -0.0024 (3) | 0.40301 (19) | 0.1745 (2) | 0.0459 (8) | |
| H14A | 0.0311 | 0.3649 | 0.1510 | 0.055* | |
| H14B | -0.0766 | 0.4188 | 0.1320 | 0.055* | |
| C15 | -0.1372 (3) | 0.44123 (17) | 0.2947 (2) | 0.0392 (8) | |
| C16 | -0.2526 (3) | 0.4525 (2) | 0.2376 (2) | 0.0612 (11) | |
| H16 | -0.2769 | 0.4292 | 0.1860 | 0.073* | |
| C17 | -0.3320 (4) | 0.4987 (2) | 0.2575 (3) | 0.0777 (13) | |
| H17 | -0.4097 | 0.5061 | 0.2192 | 0.093* | |
| C18 | -0.2964 (4) | 0.5334 (2) | 0.3334 (3) | 0.0718 (12) | |
| H18 | -0.3501 | 0.5642 | 0.3462 | 0.086* | |
| C19 | -0.1830 (4) | 0.5230 (2) | 0.3901 (3) | 0.0655 (11) | |
| H19 | -0.1593 | 0.5468 | 0.4413 | 0.079* | |
| C20 | -0.1031 (3) | 0.47681 (18) | 0.3711 (2) | 0.0512 (9) | |
| H20 | -0.0258 | 0.4696 | 0.4100 | 0.061* | |
| C21 | -0.1212 (3) | 0.29792 (17) | 0.2618 (2) | 0.0446 (8) | |
| H21A | -0.2052 | 0.3041 | 0.2255 | 0.054* | |
| H21B | -0.0824 | 0.2631 | 0.2368 | 0.054* | |
| C22 | -0.1201 (3) | 0.27699 (19) | 0.3519 (2) | 0.0500 (9) | |
| H22A | -0.1502 | 0.2307 | 0.3510 | 0.060* | |
| H22B | -0.1743 | 0.3067 | 0.3713 | 0.060* | |
| C23 | 0.0305 (3) | 0.29942 (17) | 0.5330 (2) | 0.0413 (8) | |
| C24 | -0.0603 (3) | 0.3399 (2) | 0.5480 (2) | 0.0529 (9) | |
| H24 | -0.1274 | 0.3533 | 0.5027 | 0.063* | |
| C25 | -0.0518 (4) | 0.3605 (2) | 0.6305 (3) | 0.0605 (11) | |
| H25 | -0.1135 | 0.3874 | 0.6402 | 0.073* | |
| C26 | 0.0467 (4) | 0.3415 (2) | 0.6974 (2) | 0.0590 (10) | |
| H26 | 0.0533 | 0.3564 | 0.7523 | 0.071* | |
| C27 | 0.1362 (4) | 0.3003 (2) | 0.6833 (2) | 0.0614 (11) | |
| H27 | 0.2024 | 0.2865 | 0.7290 | 0.074* | |
| C28 | 0.1287 (3) | 0.2791 (2) | 0.6017 (2) | 0.0538 (9) | |
| H28 | 0.1896 | 0.2512 | 0.5929 | 0.065* | |
| C29 | 0.1039 (3) | 0.19806 (16) | 0.42953 (19) | 0.0387 (8) | |
| C30 | 0.0425 (4) | 0.14216 (19) | 0.4497 (2) | 0.0539 (10) | |
| H30 | -0.0322 | 0.1483 | 0.4609 | 0.065* | |
| C31 | 0.0923 (5) | 0.0778 (2) | 0.4532 (3) | 0.0677 (12) | |
| H31 | 0.0515 | 0.0407 | 0.4673 | 0.081* | |
| C32 | 0.2015 (4) | 0.0680 (2) | 0.4359 (3) | 0.0675 (12) | |
| H32 | 0.2343 | 0.0244 | 0.4381 | 0.081* | |
| C33 | 0.2626 (4) | 0.1225 (2) | 0.4153 (3) | 0.0610 (11) | |
| H33 | 0.3362 | 0.1157 | 0.4029 | 0.073* | |
| C34 | 0.2149 (3) | 0.18766 (18) | 0.4131 (2) | 0.0456 (8) | |
| H34 | 0.2575 | 0.2246 | 0.4005 | 0.055* | |
| P4 | 0.33951 (10) | 0.86107 (6) | 0.53542 (7) | 0.0655 (3) | |
| F1 | 0.2344 (3) | 0.91309 (17) | 0.5407 (2) | 0.1331 (13) | |
| F2 | 0.4424 (3) | 0.81198 (16) | 0.5283 (2) | 0.1263 (12) | |
| F3 | 0.4311 (7) | 0.8949 (6) | 0.6137 (6) | 0.170 (6) | 0.614 (17) |

| | | | | | |
|-----|-------------|-------------|-------------|------------|------------|
| F4 | 0.2458 (8) | 0.8302 (5) | 0.4551 (7) | 0.181 (7) | 0.614 (17) |
| F5 | 0.3788 (11) | 0.9131 (4) | 0.4771 (7) | 0.143 (6) | 0.614 (17) |
| F6 | 0.2992 (7) | 0.8122 (5) | 0.5916 (7) | 0.196 (7) | 0.614 (17) |
| F3' | 0.3623 (16) | 0.8459 (7) | 0.6302 (5) | 0.170 (11) | 0.386 (17) |
| F4' | 0.3028 (14) | 0.8713 (10) | 0.4399 (5) | 0.184 (10) | 0.386 (17) |
| F5' | 0.4294 (9) | 0.9199 (4) | 0.5545 (15) | 0.153 (11) | 0.386 (17) |
| F6' | 0.2434 (11) | 0.8018 (5) | 0.5150 (11) | 0.141 (9) | 0.386 (17) |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|-------------|--------------|
| Pt1 | 0.02685 (7) | 0.03558 (8) | 0.03213 (7) | -0.00116 (5) | 0.00792 (5) | 0.00172 (5) |
| Cl1 | 0.0352 (4) | 0.0585 (6) | 0.0467 (5) | -0.0016 (4) | -0.0013 (4) | 0.0038 (4) |
| P1 | 0.0324 (4) | 0.0385 (5) | 0.0422 (5) | 0.0009 (4) | 0.0147 (4) | 0.0056 (4) |
| P2 | 0.0290 (4) | 0.0438 (5) | 0.0311 (4) | 0.0000 (4) | 0.0066 (3) | -0.0002 (3) |
| P3 | 0.0322 (4) | 0.0416 (5) | 0.0385 (4) | -0.0023 (4) | 0.0124 (4) | 0.0045 (4) |
| C1 | 0.0343 (17) | 0.046 (2) | 0.0465 (19) | -0.0013 (15) | 0.0144 (15) | -0.0008 (16) |
| C2 | 0.069 (3) | 0.069 (3) | 0.086 (3) | 0.022 (2) | 0.047 (3) | 0.023 (2) |
| C3 | 0.095 (4) | 0.080 (4) | 0.126 (4) | 0.042 (3) | 0.067 (4) | 0.029 (3) |
| C4 | 0.069 (3) | 0.085 (4) | 0.103 (4) | 0.011 (3) | 0.046 (3) | -0.021 (3) |
| C5 | 0.061 (3) | 0.134 (5) | 0.056 (3) | 0.015 (3) | 0.029 (2) | -0.004 (3) |
| C6 | 0.057 (2) | 0.095 (3) | 0.051 (2) | 0.021 (2) | 0.023 (2) | 0.009 (2) |
| C7 | 0.0338 (18) | 0.039 (2) | 0.064 (2) | -0.0003 (15) | 0.0188 (17) | 0.0049 (17) |
| C8 | 0.081 (3) | 0.051 (3) | 0.087 (3) | -0.012 (2) | 0.043 (3) | 0.004 (2) |
| C9 | 0.083 (3) | 0.046 (3) | 0.122 (5) | -0.012 (2) | 0.041 (3) | 0.014 (3) |
| C10 | 0.047 (2) | 0.049 (3) | 0.122 (4) | -0.014 (2) | 0.003 (3) | -0.006 (3) |
| C11 | 0.063 (3) | 0.063 (3) | 0.084 (3) | -0.006 (2) | -0.014 (2) | -0.005 (3) |
| C12 | 0.049 (2) | 0.048 (2) | 0.068 (3) | -0.0065 (18) | 0.0007 (19) | 0.0046 (19) |
| C13 | 0.0418 (19) | 0.057 (2) | 0.048 (2) | 0.0080 (17) | 0.0177 (16) | 0.0167 (17) |
| C14 | 0.0408 (18) | 0.063 (2) | 0.0335 (17) | 0.0071 (18) | 0.0111 (14) | 0.0050 (16) |
| C15 | 0.0340 (17) | 0.042 (2) | 0.0423 (18) | 0.0025 (15) | 0.0124 (15) | 0.0026 (15) |
| C16 | 0.044 (2) | 0.074 (3) | 0.058 (2) | 0.008 (2) | 0.0042 (18) | -0.010 (2) |
| C17 | 0.045 (2) | 0.084 (3) | 0.094 (3) | 0.020 (2) | 0.006 (2) | -0.006 (3) |
| C18 | 0.057 (3) | 0.064 (3) | 0.098 (3) | 0.015 (2) | 0.028 (3) | -0.015 (3) |
| C19 | 0.066 (3) | 0.063 (3) | 0.067 (3) | 0.008 (2) | 0.019 (2) | -0.017 (2) |
| C20 | 0.045 (2) | 0.052 (2) | 0.053 (2) | 0.0059 (17) | 0.0090 (17) | -0.0046 (18) |
| C21 | 0.0377 (18) | 0.044 (2) | 0.0468 (19) | -0.0053 (15) | 0.0043 (15) | -0.0068 (16) |
| C22 | 0.0346 (18) | 0.055 (2) | 0.058 (2) | -0.0089 (16) | 0.0104 (16) | 0.0066 (18) |
| C23 | 0.0398 (18) | 0.045 (2) | 0.0432 (18) | -0.0014 (15) | 0.0189 (15) | 0.0061 (15) |
| C24 | 0.047 (2) | 0.063 (2) | 0.051 (2) | 0.0083 (19) | 0.0199 (18) | 0.0037 (19) |
| C25 | 0.060 (3) | 0.069 (3) | 0.062 (3) | 0.009 (2) | 0.032 (2) | 0.000 (2) |
| C26 | 0.076 (3) | 0.062 (3) | 0.046 (2) | 0.002 (2) | 0.027 (2) | 0.0018 (19) |
| C27 | 0.067 (3) | 0.073 (3) | 0.042 (2) | 0.012 (2) | 0.0129 (19) | 0.0082 (19) |
| C28 | 0.055 (2) | 0.062 (3) | 0.046 (2) | 0.0145 (19) | 0.0190 (18) | 0.0076 (18) |
| C29 | 0.0413 (18) | 0.040 (2) | 0.0339 (16) | -0.0049 (15) | 0.0096 (14) | 0.0008 (14) |
| C30 | 0.060 (2) | 0.053 (3) | 0.051 (2) | -0.0172 (19) | 0.0205 (19) | -0.0012 (18) |
| C31 | 0.096 (4) | 0.043 (3) | 0.061 (3) | -0.020 (2) | 0.020 (2) | 0.0018 (19) |
| C32 | 0.086 (3) | 0.042 (2) | 0.063 (3) | 0.008 (2) | 0.005 (2) | -0.007 (2) |

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|-----|------------|------------|------------|--------------|-------------|-------------|
| C33 | 0.057 (2) | 0.053 (3) | 0.069 (3) | 0.007 (2) | 0.012 (2) | -0.007 (2) |
| C34 | 0.045 (2) | 0.043 (2) | 0.049 (2) | -0.0006 (16) | 0.0130 (16) | 0.0008 (16) |
| P4 | 0.0518 (6) | 0.0859 (9) | 0.0608 (7) | 0.0022 (6) | 0.0199 (5) | 0.0198 (6) |
| F1 | 0.085 (2) | 0.135 (3) | 0.193 (4) | 0.031 (2) | 0.062 (2) | 0.027 (3) |
| F2 | 0.100 (2) | 0.108 (3) | 0.178 (3) | 0.0275 (19) | 0.052 (2) | -0.005 (2) |
| F3 | 0.082 (5) | 0.309 (16) | 0.115 (7) | -0.058 (7) | 0.025 (4) | -0.069 (8) |
| F4 | 0.133 (9) | 0.174 (11) | 0.166 (11) | 0.000 (7) | -0.061 (7) | -0.044 (8) |
| F5 | 0.200 (12) | 0.121 (8) | 0.155 (10) | 0.039 (7) | 0.122 (9) | 0.062 (7) |
| F6 | 0.121 (6) | 0.265 (13) | 0.210 (13) | -0.036 (7) | 0.061 (8) | 0.170 (11) |
| F3' | 0.27 (3) | 0.174 (15) | 0.051 (5) | 0.124 (16) | 0.023 (9) | 0.000 (7) |
| F4' | 0.183 (16) | 0.31 (3) | 0.047 (6) | -0.042 (14) | 0.010 (8) | 0.053 (10) |
| F5' | 0.083 (8) | 0.077 (7) | 0.31 (3) | -0.036 (5) | 0.079 (15) | -0.040 (13) |
| F6' | 0.163 (15) | 0.110 (10) | 0.198 (19) | -0.074 (10) | 0.130 (15) | -0.031 (10) |

Geometric parameters (Å, °)

| | | | |
|---------|------------|----------|-----------|
| Pt1—P2 | 2.2095 (8) | C17—C18 | 1.371 (6) |
| Pt1—P3 | 2.3007 (8) | C17—H17 | 0.9300 |
| Pt1—P1 | 2.3185 (8) | C18—C19 | 1.361 (6) |
| Pt1—C11 | 2.3434 (8) | C18—H18 | 0.9300 |
| P1—C7 | 1.814 (4) | C19—C20 | 1.384 (5) |
| P1—C1 | 1.819 (3) | C19—H19 | 0.9300 |
| P1—C13 | 1.836 (3) | C20—H20 | 0.9300 |
| P2—C15 | 1.812 (3) | C21—C22 | 1.535 (5) |
| P2—C21 | 1.815 (3) | C21—H21A | 0.9700 |
| P2—C14 | 1.828 (3) | C21—H21B | 0.9700 |
| P3—C23 | 1.812 (3) | C22—H22A | 0.9700 |
| P3—C29 | 1.817 (3) | C22—H22B | 0.9700 |
| P3—C22 | 1.848 (3) | C23—C24 | 1.383 (5) |
| C1—C2 | 1.380 (5) | C23—C28 | 1.387 (5) |
| C1—C6 | 1.389 (5) | C24—C25 | 1.392 (5) |
| C2—C3 | 1.381 (6) | C24—H24 | 0.9300 |
| C2—H2 | 0.9300 | C25—C26 | 1.365 (6) |
| C3—C4 | 1.359 (6) | C25—H25 | 0.9300 |
| C3—H3 | 0.9300 | C26—C27 | 1.375 (5) |
| C4—C5 | 1.362 (6) | C26—H26 | 0.9300 |
| C4—H4 | 0.9300 | C27—C28 | 1.382 (5) |
| C5—C6 | 1.388 (6) | C27—H27 | 0.9300 |
| C5—H5 | 0.9300 | C28—H28 | 0.9300 |
| C6—H6 | 0.9300 | C29—C34 | 1.385 (4) |
| C7—C12 | 1.381 (5) | C29—C30 | 1.393 (5) |
| C7—C8 | 1.390 (5) | C30—C31 | 1.379 (5) |
| C8—C9 | 1.390 (6) | C30—H30 | 0.9300 |
| C8—H8 | 0.9300 | C31—C32 | 1.370 (6) |
| C9—C10 | 1.352 (7) | C31—H31 | 0.9300 |
| C9—H9 | 0.9300 | C32—C33 | 1.372 (6) |
| C10—C11 | 1.375 (6) | C32—H32 | 0.9300 |
| C10—H10 | 0.9300 | C33—C34 | 1.385 (5) |
| C11—C12 | 1.386 (5) | C33—H33 | 0.9300 |

| | | | |
|------------|-------------|---------------|-----------|
| C11—H11 | 0.9300 | C34—H34 | 0.9300 |
| C12—H12 | 0.9300 | P4—F6 | 1.496 (5) |
| C13—C14 | 1.535 (5) | P4—F5' | 1.512 (8) |
| C13—H13A | 0.9700 | P4—F4' | 1.512 (8) |
| C13—H13B | 0.9700 | P4—F3' | 1.530 (8) |
| C14—H14A | 0.9700 | P4—F3 | 1.542 (7) |
| C14—H14B | 0.9700 | P4—F2 | 1.548 (3) |
| C15—C16 | 1.383 (5) | P4—F4 | 1.549 (6) |
| C15—C20 | 1.387 (5) | P4—F5 | 1.556 (6) |
| C16—C17 | 1.387 (5) | P4—F6' | 1.563 (8) |
| C16—H16 | 0.9300 | P4—F1 | 1.595 (3) |
| P2—Pt1—P3 | 85.22 (3) | C18—C19—C20 | 119.7 (4) |
| P2—Pt1—P1 | 85.71 (3) | C18—C19—H19 | 120.1 |
| P3—Pt1—P1 | 167.13 (3) | C20—C19—H19 | 120.1 |
| P2—Pt1—C11 | 175.83 (3) | C19—C20—C15 | 120.7 (3) |
| P3—Pt1—C11 | 91.79 (3) | C19—C20—H20 | 119.7 |
| P1—Pt1—C11 | 97.69 (3) | C15—C20—H20 | 119.7 |
| C7—P1—C1 | 108.56 (15) | C22—C21—P2 | 107.0 (2) |
| C7—P1—C13 | 104.36 (16) | C22—C21—H21A | 110.3 |
| C1—P1—C13 | 105.78 (16) | P2—C21—H21A | 110.3 |
| C7—P1—Pt1 | 119.51 (12) | C22—C21—H21B | 110.3 |
| C1—P1—Pt1 | 111.53 (12) | P2—C21—H21B | 110.3 |
| C13—P1—Pt1 | 105.99 (11) | H21A—C21—H21B | 108.6 |
| C15—P2—C21 | 105.12 (16) | C21—C22—P3 | 110.3 (2) |
| C15—P2—C14 | 107.82 (16) | C21—C22—H22A | 109.6 |
| C21—P2—C14 | 113.75 (16) | P3—C22—H22A | 109.6 |
| C15—P2—Pt1 | 114.03 (11) | C21—C22—H22B | 109.6 |
| C21—P2—Pt1 | 108.04 (11) | P3—C22—H22B | 109.6 |
| C14—P2—Pt1 | 108.22 (11) | H22A—C22—H22B | 108.1 |
| C23—P3—C29 | 106.08 (15) | C24—C23—C28 | 118.9 (3) |
| C23—P3—C22 | 109.46 (16) | C24—C23—P3 | 122.1 (3) |
| C29—P3—C22 | 106.05 (16) | C28—C23—P3 | 118.4 (3) |
| C23—P3—Pt1 | 114.22 (11) | C23—C24—C25 | 120.3 (4) |
| C29—P3—Pt1 | 113.54 (11) | C23—C24—H24 | 119.9 |
| C22—P3—Pt1 | 107.16 (11) | C25—C24—H24 | 119.9 |
| C2—C1—C6 | 118.3 (3) | C26—C25—C24 | 120.4 (4) |
| C2—C1—P1 | 120.0 (3) | C26—C25—H25 | 119.8 |
| C6—C1—P1 | 121.6 (3) | C24—C25—H25 | 119.8 |
| C1—C2—C3 | 120.9 (4) | C25—C26—C27 | 119.7 (4) |
| C1—C2—H2 | 119.6 | C25—C26—H26 | 120.1 |
| C3—C2—H2 | 119.6 | C27—C26—H26 | 120.1 |
| C4—C3—C2 | 120.1 (4) | C26—C27—C28 | 120.6 (4) |
| C4—C3—H3 | 120.0 | C26—C27—H27 | 119.7 |
| C2—C3—H3 | 120.0 | C28—C27—H27 | 119.7 |
| C3—C4—C5 | 120.4 (4) | C27—C28—C23 | 120.2 (3) |
| C3—C4—H4 | 119.8 | C27—C28—H28 | 119.9 |
| C5—C4—H4 | 119.8 | C23—C28—H28 | 119.9 |
| C4—C5—C6 | 120.2 (4) | C34—C29—C30 | 118.9 (3) |
| C4—C5—H5 | 119.9 | C34—C29—P3 | 121.6 (3) |

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|---------------|-----------|-------------|-----------|
| C6—C5—H5 | 119.9 | C30—C29—P3 | 119.5 (3) |
| C5—C6—C1 | 120.1 (4) | C31—C30—C29 | 120.1 (4) |
| C5—C6—H6 | 119.9 | C31—C30—H30 | 120.0 |
| C1—C6—H6 | 119.9 | C29—C30—H30 | 120.0 |
| C12—C7—C8 | 119.1 (4) | C32—C31—C30 | 120.5 (4) |
| C12—C7—P1 | 119.7 (3) | C32—C31—H31 | 119.8 |
| C8—C7—P1 | 121.1 (3) | C30—C31—H31 | 119.8 |
| C7—C8—C9 | 119.5 (4) | C31—C32—C33 | 120.1 (4) |
| C7—C8—H8 | 120.3 | C31—C32—H32 | 119.9 |
| C9—C8—H8 | 120.3 | C33—C32—H32 | 119.9 |
| C10—C9—C8 | 121.0 (4) | C32—C33—C34 | 120.1 (4) |
| C10—C9—H9 | 119.5 | C32—C33—H33 | 119.9 |
| C8—C9—H9 | 119.5 | C34—C33—H33 | 119.9 |
| C9—C10—C11 | 119.9 (4) | C29—C34—C33 | 120.3 (3) |
| C9—C10—H10 | 120.0 | C29—C34—H34 | 119.9 |
| C11—C10—H10 | 120.0 | C33—C34—H34 | 119.9 |
| C10—C11—C12 | 120.2 (5) | F5'—P4—F4' | 94.2 (8) |
| C10—C11—H11 | 119.9 | F5'—P4—F3' | 92.3 (7) |
| C12—C11—H11 | 119.9 | F4'—P4—F3' | 173.1 (8) |
| C7—C12—C11 | 120.2 (4) | F6—P4—F3 | 90.9 (5) |
| C7—C12—H12 | 119.9 | F6—P4—F2 | 91.6 (4) |
| C11—C12—H12 | 119.9 | F5'—P4—F2 | 90.6 (4) |
| C14—C13—P1 | 110.6 (2) | F4'—P4—F2 | 89.0 (5) |
| C14—C13—H13A | 109.5 | F3'—P4—F2 | 93.2 (4) |
| P1—C13—H13A | 109.5 | F3—P4—F2 | 89.6 (4) |
| C14—C13—H13B | 109.5 | F6—P4—F4 | 90.9 (5) |
| P1—C13—H13B | 109.5 | F3—P4—F4 | 177.5 (5) |
| H13A—C13—H13B | 108.1 | F2—P4—F4 | 92.0 (3) |
| C13—C14—P2 | 106.3 (2) | F6—P4—F5 | 178.6 (5) |
| C13—C14—H14A | 110.5 | F3—P4—F5 | 89.1 (4) |
| P2—C14—H14A | 110.5 | F2—P4—F5 | 89.8 (3) |
| C13—C14—H14B | 110.5 | F4—P4—F5 | 89.0 (5) |
| P2—C14—H14B | 110.5 | F5'—P4—F6' | 178.3 (6) |
| H14A—C14—H14B | 108.7 | F4'—P4—F6' | 85.3 (8) |
| C16—C15—C20 | 118.9 (3) | F3'—P4—F6' | 88.1 (6) |
| C16—C15—P2 | 120.1 (3) | F2—P4—F6' | 91.0 (4) |
| C20—C15—P2 | 120.9 (3) | F6—P4—F1 | 90.1 (4) |
| C15—C16—C17 | 119.9 (4) | F5'—P4—F1 | 88.4 (4) |
| C15—C16—H16 | 120.1 | F4'—P4—F1 | 89.7 (5) |
| C17—C16—H16 | 120.1 | F3'—P4—F1 | 88.2 (4) |
| C18—C17—C16 | 120.2 (4) | F3—P4—F1 | 90.5 (4) |
| C18—C17—H17 | 119.9 | F2—P4—F1 | 178.3 (2) |
| C16—C17—H17 | 119.9 | F4—P4—F1 | 87.8 (3) |
| C19—C18—C17 | 120.6 (4) | F5—P4—F1 | 88.5 (3) |
| C19—C18—H18 | 119.7 | F6'—P4—F1 | 90.0 (4) |
| C17—C18—H18 | 119.7 | | |

Fig. 1

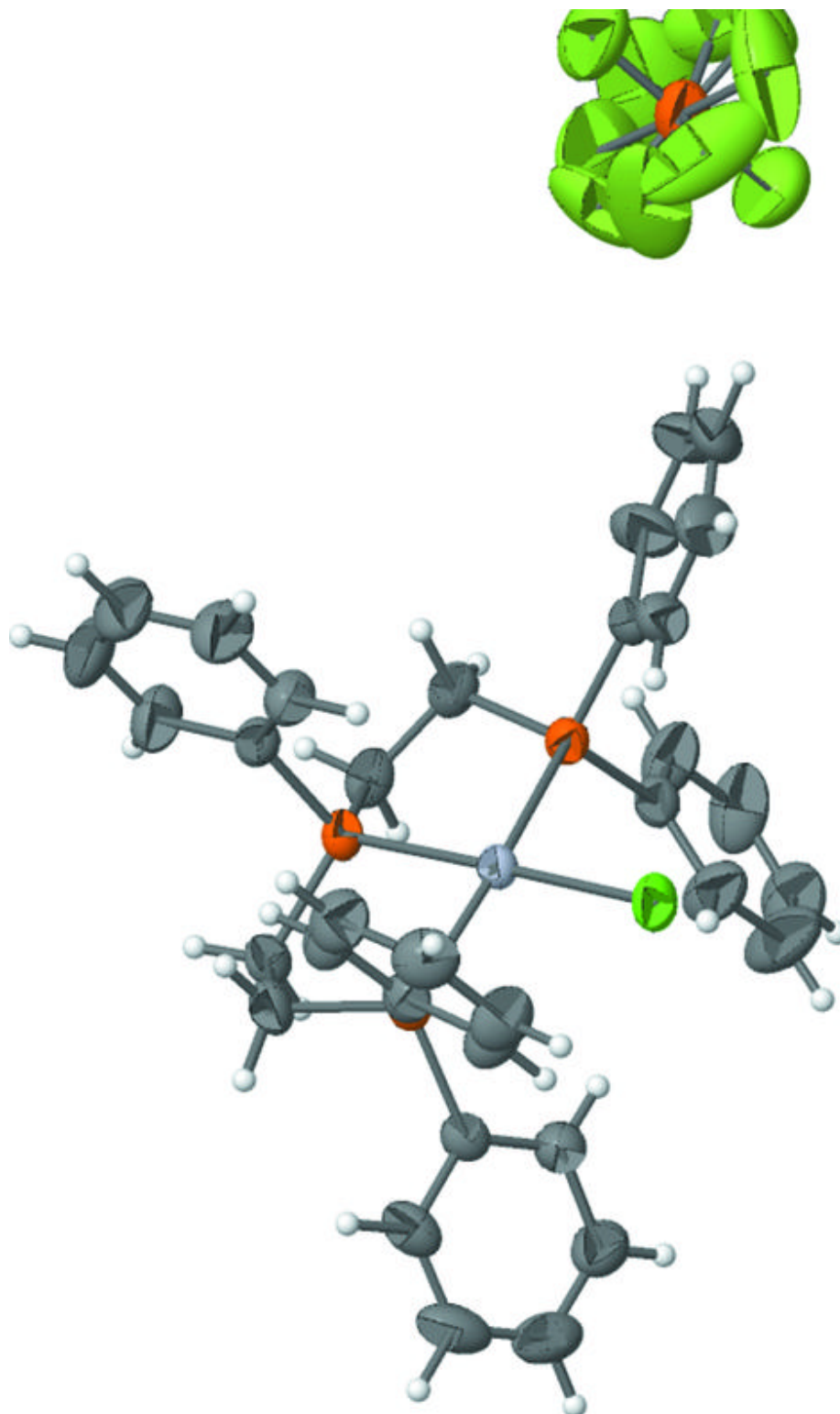


Fig. 2

